REPORT DOCUMENTATION PAGE	Form Approved OMB No. 0704-0188

1. REPORT DATE ***(DD-MM-YYYY)***	**2. REPORT TYPE**	**3. DATES COVERED** *(From – To)*
18-11-2003	Conference Proceedings	27 July 2003 - 30 July 2003

4. TITLE AND SUBTITLE Workshop on Quantification of Microstructure and the Linkage to Property Modeling	**5a. CONTRACT NUMBER** FA8655-03-M5051
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S) Conference Committee	**5d. PROJECT NUMBER**
	5d. TASK NUMBER
	5e. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Best Western Hotel Hofgut Sternen Höllsteig 76 Breitnau D-79874 Germany	**8. PERFORMING ORGANIZATION REPORT NUMBER** N/A
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) EOARD PSC 802 BOX 14 FPO 09499-0014	**10. SPONSOR/MONITOR'S ACRONYM(S)**
	11. SPONSOR/MONITOR'S REPORT NUMBER(S) CSP 03-5051

12. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

20040715 189

14. ABSTRACT

The Final Proceedings for Workshop on Quantification of Microstructure and the Linkage to Property Modeling, 27 July 2003 - 30 July 2003

The objective of this workshop is to review recent advances in the characterization and representation of microstructure within mechanical property models. Topics to be addressed include new approaches to three-dimensional quantification of material structure across all relevant length scales and the use of microstructural parameters in monotonic, cyclic and time dependent property models. Other topics of potential interest include probabilistic aspects of property prediction, microstructurally-informed constitutive modeling, crystal plasticity approaches and representation of key aspects of microstructure within continuum finite element models.

15. SUBJECT TERMS

EOARD, Modeling & Simulation, Metals & alloys, Dislocation theory, Microstructure, Mesoscale

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18, NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			CHARLES H. WARD, Lt Col, USAF
UNCLAS	UNCLAS	UNCLAS	UL	3	**19b. TELEPHONE NUMBER** *(Include area code)* +44 (0)20 7514 3154

Workshop Report
Quantification of Microstructure and the Linkage to Property Modeling
27–30 July 2003, Breitnau (Freiburg), Germany

A workshop was held to provide a forum for discussions among research scientists that explored the current status of European research on microstructural characterization and microstructure-explicit modeling of the mechanical behavior of materials. The workshop was structured in five half-day sessions that evolved from the more fundamental to engineering applications.

Session 1 was devoted to *Technological requirements and definition of microstructure.* Presentations by Dr. Craig Hartley (AFOSR), Prof. Hamish Fraser (The Ohio State Univ.) and Prof. Peter Gumbsch (Fraunhofer Institute, Freiburg) outlined the current philosophies to accelerating the introduction of novel materials into complex applications. Prof. Phil Withers (University of Manchester) and Prof. Tony Rollett (Carnegie-Mellon Univ.) gave papers on advances in the experimental and theoretical characterization of materials microstructure. Prof. Fraser's presentation illustrated the power of employing 'rules-based' methods (neural networks, etc.) to elucidate important microstructural variables for materials that are not we understood, although there was much discussion about the limited ability to extrapolate from these methods. Prof. Gumbsch emphasized the role of modeling in design, but suggested that even those models once considered of an academic nature, such as atomistic models, are the actual design models for the nano-technology world. He further showed that robust tools are need to fit model parameters and that optimization sciences are important for this. Prof. Withers emphasized that new 3D x-ray characterization methods, and 2D strain field mapping will change the accuracy and fidelity of experiments in the deformation sciences, thus permitting access to microstructural influences. Finally, Prof. Rollett suggested that theory implies an opportunity for defining interface properties and using these in kinetics models; however, practical studies indicate that this has not been achieved and greater scientific understanding is needed.

Session 2 was devoted to *Dislocation activity – from fundamentals to constitutive descriptions.* Presentations by Prof. Michael Zaiser (University of Edinburgh) and Dr. Ladislas Kubin (ONERA) gave alternative accounts of the links between fundamental approaches to dislocation dynamics and constitutive model of crystal plasticity. Prof. Dierk Raabe (MPI, Düsseldorf) gave a complementary paper on experimental characterization of crystal plasticity related to simulations of bulk and interface micromechanics. Prof. Franz-Dieter Fischer (Montan Univ., Leoben) dealt with experiments and modeling of deformation twinning. Prof. Zaiser's work illustrated the need to ties discrete dislocation behavior to continuum strain-gradient theories, and that the ties exist in the domains of correlation functions and probability functions for dislocation aggregate behavior. Dr. Kubin re-capped his more than a decade of studies using discrete dislocation simulations, but indicated that basic understanding of dislocation patterning is still lacking. Nonetheless he showed good progress with establishing a continuum 'hardening matrix' that proves rather useful in representing single-crystal deformation anisotropy. Prof. Fischer illustrated the use of a continuum method to treat deformation twinning and showed that such a method is well founded from energy principles. Perhaps the highlight of the session was Prof. Raabe's description of coupled continuum modeling and direct experiments which showed the critical importance of capturing polycrystalline kinematics for accurate deformation predictions.

AQ F04-09-0999

The theme of Session 3 was *Microstructure/property relationships and multiscale modeling* in which the microstructure is relatively stable. Prof. Tresa Pollock (University of Michigan) dealt with microstructural-scale plastic heterogeneity in high temperature materials concentrating on novel approaches to property and microstructural characterization. Dr. T. Parthasarathy (UES, Inc) described advances in computer simulation of the microstructural dependence of strength for superalloys. Prof. Esteban Busso (Imperial College) discussed how theoretical treatments at different microstructural scales could be incorporated in constitutive formulations for materials with heterogeneous microstructures. Prof. Oliver Kraft (Forshungszentrum Karlsruhe) discussed the effect of grain size and film thickness on cyclic deformation and fatigue in thin metal film. Prof. Hael Mughrabi (University of Erlangen) reviewed the phenomenology of microstructural instabilities on different length scales in cyclically deformed metals. Prof. Pollock's presentation illustrated power of using 2D strain-filed mapping in experimentally verifying the microstructural effects in models. She further suggested that future development of the method may be important for validating strain-gradient plasticity approaches. Dr. Parthasarathy presented a systematic framework for linking discrete-dislocation simulations with material microstructural images or synthetically-derived microstructures to produce response surfaces for microstructural effects on deformation. He further shows the engineering importance of such a method for both defining materials parameters in finite-element simulations and for building 'fast-acting' spread-sheet models for engineering design. Prof. Busso reported on a multiscale approach for simulating the turbine-engine single-crystal airfoils. He suggested criteria for defining 'representative volume elements' based on material parameters, and showed the use of strain-gradient theory to represent microstructural effects on superalloy deformation. Prof. Kraft then described microstructural effects on deformation at dramatically different length and time scales as he showed results from fatigue of nano-meter scale Cu thin films tested at Giga-Hz frequencies. The works shows what may be a break-down of parabolic scaling of the dislocation density with strain, although the test conditions require such that further validation is needed. Finally, Prof. Mughrabi showed that even topics that are considered mature, such as the basic stages of single crystal deformation and aspects of strain hardening, require complete re-evaluation once nano-crystalline scale microstructures are considered. Such materials show dramatic extensions of Stage I behavior, followed by catastrophic breakdown and failure in Stage III for nanocrystalline materials.

Session 4 was devoted to *Multiscale modeling with evolving damage and microstructure,* which predominantly occurs during long duration/ high temperature service conditions where creep is often life-limiting. Prof. Brian Dyson (Imperial College) presented a microstructure-explicit quantitative model of creep in precipitation-strengthened alloys. Dr. Fionn Dunne (University of Oxford) described a similar approach to modeling creep and fatigue in a nickel-base superalloy in which the strengthening precipitate dissolves at the higher service temperatures. Prof. Malcolm McLean (Imperial College) complemented the creep modeling by pointing to the value of diagnostic testing, including cauterization of crystal rotations in singled crystals, to unambiguously identify the operative damage mechanisms. Prof. Gunther Eggeler (University of Bochum) discussed recent progress in understanding the role of microstructure in controlling creep in single crystal superalloys at high temperature and low stress. Prof. Dyson's worked showed that power of continuum damage mechanics for representing a wide variety of microstructurally-influenced creep responses for materials, but further illustrated how such methods are limited by a need for a comprehensive database. Gunther Eggeler suggested that

microstructurally-based modeling for creep performance will not progress too rapidly without further description and understanding to the dislocation-level processes that lead to the defeat of reinforcing particles during creep straining. He described his continuing careful efforts to understand such phenomena using his novel double-shear specimen configuration. Dr. Dunne introduced the idea of "critical accumulated slip" for fatigue crack initiation modeling and showed that many aspects of fatigue behavior are well represented with a simple two-parameter model. However, the model needs further development within a finite element framework if triaxial microstructural stresses are to be captured. Finally, Prof McClean closed the session with a talk that illustrated the challenges that materials such as the nickel-based superalloys present for creep modeling. His work has shown that the materials actually shrink during tensile loading over an important part of the temperature and time regime for engineering use of the alloys. Such behavior has never been considered in creep modeling and is not well understood from a mechanistic level.

The final session was on *Engineering applications and future requirements.* Dr. Hermann Riedel (Fraunhofer Institute Freiburg) described the simulation of powder metallurgical processing incorporating microstructural evolution. Prof. David Hayhurst (University of Manchester) discussed the links between microstructure/physical mechanisms and the selection of constitutive equations for use within a high-temperature continuum damage mechanics framework, that have the ability to predict damage initiation and creep crack growth in engineering components. Dr. Dennis Dimiduk (AFRL/MLLM) concluded the formal program with a presentation on Air Force activities on Accelerated Insertion of Materials (AIM). Prof. Riedel showed the continued utility of standard state-variable descriptions for engineering design, but illustrated that the quality of such approached is tied to the availability of data. Similarly, Prof. Hayhurst showed that when data that satisfy key microstructural responses are available, the continuum damage method for creep modeling permits representation of transitions between fundamentally different damage process over the full duration of creep lifetimes.

Dr. Dimiduk's presentation provided an overall contest for the subject matter of workshop by suggesting future directions and nearer-term challenges for microstructurally-based modeling for design. His work described the grander vision being supported by the Defense Advanced Research Projects Agency's "Accelerated Insertion of Materials" effort, and he outlined a methodology for establishing a microstructurally based predictive capability for material behavior. The talk illustrated the excitement and technical challenges that motivated this workshop and are drawing growing focus to this area of science and engineering.

In summary, many participants in the workshop departed with a better -defined vision for the future. Several counted the interactions at the workshop as some of the most fruitful that they had been a part of for a some time, and suggested that such workshops fill a role for scientific interchange that cannot be accomplished though other meetings and professional society gatherings.